

Does mesoscopic disorder imply microscopic chaos?

Peter Grassberger and Thomas Schreiber

Physics Department, University of Wuppertal, Germany

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We argue that Gaspard and coworkers [1] do not give evidence for microscopic chaos in the sense in which they use the term. The effectively infinite number of molecules in a fluid can generate the same macroscopic disorder without any intrinsic instability. But we argue also that the notion of chaos in infinitely extended systems needs clarification: In a wider sense, even some systems without local instabilities can be considered chaotic.

In a beautiful recent experiment [1], Gaspard and coworkers verified that the position of a Brownian particle behaves like a Wiener process with positive resolution dependent entropy [3]. More surprisingly and dramatically [2], they claim that this observation gives a first proof of “microscopic chaos”, a term they illustrate by examples of finite dimensional dynamical systems which are intrinsically unstable. While the recent literature finds such chaos on a molecular level quite plausible, we argue that the observed macroscopic disorder cannot be taken as direct evidence. In fact, Brownian motion can be derived for systems which would usually be called non-chaotic, think of a tracer particle in a non-interacting ideal gas. All that is needed for diffusion is *molecular chaos* in the sense of Boltzmann, i.e. the absence of observable correlations in the motion of single molecules.

Part of the confusion is due to the lack of a unique definition of “microscopic chaos” for systems with infinitely many degrees of freedom. The authors of [1] introduce the term by extrapolating finite dimensional dynamical systems for which chaos is a well defined concept: Initially close states on average separate exponentially when time goes to infinity. The rate of separation, the Lyapunov exponent, is independent of the particular method to measure “closeness”. However, the notions of diffusion and Brownian motion involve by necessity infinitely many degrees of freedom. In this thermodynamic limit, Lyapunov exponents are no longer independent of the metric. As a consequence, the large system limit of a finite non-chaotic system will remain non-chaotic with one particular metric and become chaotic with another.

Let us illustrate this astonishing fact with an example introduced by Wolfram [4] in the

context of cellular automata. Consider two states $\mathbf{x} = (\dots x_{-2}, x_{-1}, x_0, x_1, x_2 \dots)$ and $\mathbf{y} = (\dots y_{-2}, y_{-1}, y_0, y_1, y_2 \dots)$ of a one-dimensional bi-infinite lattice system. If the distance between \mathbf{x} and \mathbf{y} is defined by $d_{\max}(\mathbf{x}, \mathbf{y}) = \max_i |x_i - y_i|$, it can grow exponentially only if the local differences do. This is what one usually means by “chaos”, and this is what the authors of [1] had meant by “microscopic chaos”. This mechanism is absent in the thermodynamic limit of finite non-chaotic systems. Therefore, some authors [5] would also call the limit non-chaotic. However, the metric $d_{\exp}(\mathbf{x}, \mathbf{y}) = \sum_i |x_i - y_i| e^{-|i|}$ can also show exponential divergence if an initially far away perturbation just moves towards the origin without growing [4]. Arguably, when observing a localised tracer like in [1], the latter choice of metric seems more appropriate.

In finite dimensional dynamical systems, chaos arises due to the de-focusing microscopic dynamics. The positive entropy is generated by the initially insignificant digits of the initial condition which are brought forth by the dynamics. In the thermodynamic limit, also a completely different mechanism exists: Perturbations coming from far away regions kick the tracer particle once and move again away to infinity. The entropy is positive due to information stored in remote parts of the initial condition. Associated to this, one can also define suitable Lyapunov exponents [4].

To resolve the confusion, we suggest to follow Sinai [6] and first let the system size tend to infinity, and only then the observation time. In that case, a system observed in a particular metric μ is called μ -chaotic when we find a positive Lyapunov exponent using this metric. However, Gaspard et al. had obviously in mind the type of chaos detectable with the metric d_{\max} , and arising from a local instability. For this, they fall short of giving experimental evidence.

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